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Pedotransfer functions: bridging the gap between available basic soil data and missing soil hydraulic characteristics

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Abstract

Water retention and hydraulic conductivity are crucial input parameters in any modelling study on water flow and solute transport in soils. Due to inherent temporal and spatial variability in these hydraulic characteristics, large numbers of samples are required to properly characterise areas of land. Hydraulic characteristics can be obtained from direct laboratory and field measurements. However, these measurements are time consuming which makes it costly to characterise an area of land. As an alternative, analysis of existing databases of measured soil hydraulic data may result in pedotransfer functions. In practise, these functions often prove to be good predictors for missing soil hydraulic characteristics. Examples are presented of different equations describing hydraulic characteristics and of pedotransfer functions used to predict parameters in these equations. Grouping of data prior to pedotransfer function development is discussed as well as the use of different soil properties as predictors. In addition to regression analysis, new techniques such as artificial neural networks, group methods of data handling, and classification and regression trees are increasingly being used for pedotransfer function development. Actual development of pedotransfer functions is demonstrated by describing a practical case study. Examples are presented of pedotransfer function for predicting other than hydraulic characteristics. Accuracy and reliability of pedotransfer functions are demonstrated and discussed. In this respect, functional evaluation of pedotransfer functions proves to be a good tool to assess the desired accuracy of a pedotransfer function for a specific application.

Keywords: Soil process modelling; Simulation; Regression; Neural network; Accuracy; Reliability; Functional evaluation

1. Introduction

To monitor and manage transport of chemicals in soils, sophisticated models are developed to describe how water and dissolved compounds move into and through soil. Studies of possible global climate change rely on numerical models that simulate heat and water fluxes at the soil surface. Hydrological models are used to partition precipitation in runoff and infiltration, and to calculate evapotranspiration. These different types of models have become indispensable tools in research directed towards quantifying and integrating the most important physical, chemical and biological processes active in the unsaturated zone of soils. Use of models for research and management requires input parameters governing retention and transport of water and chemicals in soils. At the same time these data are usually fragmented, of different degrees of detail, of varying reliability and are held in different institutes scattered throughout the world. In addition, temporal and spatial variability in hydraulic characteristics have a significant effect on model results. The characteristics

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vary from one location to the other while cultivation practices, shrink and swell phenomena, and soil crusting also cause the characteristics to vary in time. Also variations in biological activity are significant both through the blockage of pores by new roots during the growing season and through blockages associated with microbial activity. Likewise, water repellence can have an important influence on hydraulic characteristics even in non-sandy soils.

Despite the progress that is being made in direct measurement of the hydraulic characteristics, the majority of these techniques remain relatively time-consuming and therefore costly. At the same time, good predictions instead of direct measurements may be accurate enough for many applications. Therefore, the need to make new measurements has to be critically evaluated, considering both the desired accuracy and the available financial resources. As a consequence, it is rewarding to analyse existing databases containing measured data in such a way that hydraulic characteristics are predicted from available measured soil data.

Following Briggs and Shantz (1912), who were the pioneers in the field, generations of researchers quantified and interpreted relationships between available and missing soil properties. Notably McKeague et al. (1984) made an important contribution by reviewing activities in different countries and by providing a focus for subsequent research. Terms such as *predicting soil properties*, *estimating soil properties*, and *correlating soil properties*, were used interchangeably to name contents, procedures and results of such studies (Rawls et al., 1991; Van Genuchten and Leij, 1992; Pachepsky et al., 1999). In essence they all describe predictive functions that translate data *we have* into data *we need*.

Statistical regression equations, expressing relationships between soil properties, were proposed to be called *transfer functions* (Bouma and van Lanen, 1987) and later *pedotransfer functions* (PTFs) (Bouma, 1989; Hamblin, 1991). Predicting soil hydraulic characteristics dominates the research field, although soil chemical and biological characteristics are also being predicted. Several reviews on PTF development and its use have been published (e.g. Rawls et al., 1991; Van Genuchten and Leij, 1992; Timlin et al., 1996; Wösten, 1997; Pachepsky et al., 1999). Large databases, such as UNSODA (Leij et al., 1996), HYPRES (Lilly, 1997; Wösten et al., 1999), WISE (Batjes, 1996), and USDA Natural Resource Conservation Service pedon database (USDA Natural Resource Conservation Service, 1994), are available for development of PTFs.

The apparent easiness of developing PTFs should not overshadow several basic questions that need to be answered by hydrologists and soil scientists. In this respect, relevant questions are:

- How can the accuracy and reliability of PTFs be quantified?
- What is the desired accuracy and reliability of PTFs in relation to other sources of uncertainty?
- What are the most appropriate techniques to evaluate a PTF?
- What input variables are more preferable or necessary to be included in a PTF?

An inventory of existing PTFs can help to start answering these questions in a systematic fashion. The objective of this paper is to review the current status of PTF development, their uncertainty and their practical use in modelling. In this paper, accuracy of a PTF is broadly defined as the correspondence between measured and predicted data for the data set *from which a PTF has been developed*. Reliability of PTF is assessed in terms of correspondence between measured and predicted data for the data set *other than the one used to develop a PTF*. Finally, the utility of PTFs in modelling is defined as the correspondence between *measured and simulated functional soil behavior*.

2. Indirect methods for predicting hydraulic characteristics

In the context of this paper, indirect methods refer to an approach in which hydraulic characteristics are not directly measured, but predicted from data recorded in soil surveys such as percentages clay, silt and organic matter or data on particle size distribution or water retention. Since properties recorded in soil surveys show spatial variability within mapping units, it is important to not restrict application of PTFs to representative profiles and associated representative soil properties only, but to also take into account

spatial variability. In Section 11, a case study is presented that explicitly deals with spatial variability of soil properties. It should be noted that no indirect methods exist without direct methods because only direct measurements will create the required database for derivation and calibration of predicted hydraulic characteristics. Therefore, development of indirect methods implies that continued research towards accurate, up-to-date and efficient direct measurement techniques is very relevant. Availability of measured hydraulic characteristics for a wide range of different soils and accessibility of these characteristics from large and reliable international databases are, therefore, absolute prerequisites for the development of pedotransfer functions.

When using the indirect method or pedotransfer approach, three different types of PTF can be distinguished.

2.1. Type 1: Predicting hydraulic characteristics based on a soil structure model

Bloemen (1980), Arya and Paris (1981) and Arya and Dierolf (1992) presented models to predict water retention from information on particle-size distribution, bulk density and particle density. This type of models first translates particle-size distribution into an equivalent pore-size distribution model, which in turn, is related to a distribution of water contents and associated pressure heads. In these models, use is made of similarity in shape between the water retention curve and the cumulative particle-size distribution. The Arya–Paris model which has been modified and extended by several investigators (e.g. Haverkamp and Parlange, 1986; Tyler and Wheatcraft, 1988) predicts water retention characteristics for sandy soils that compare well with measured data. However, agreement between predicted and measured data for loamy and clayey soils is worse. If at least one point of the hydraulic conductivity characteristic is measured, complete conductivity characteristics can be predicted in a similar way from water retention characteristics. In this approach, the measured water retention curve is described with an analytical function. Based on this, a pore size distribution is derived which, in turn, is used to predict a hydraulic conductivity function assuming water flow through cylindrical soil pores. Mualem (1992) showed that there are a number of methods for predicting unsaturated hydraulic conductivity from measured water retention data. Among these methods, approaches related to theories of Childs and Collis-George (1950), Burdine (1953) and Mualem (1976) are widely used. The concept of soils consisting of bundles of cylindrical pores is a simplified one. Therefore, predictions of hydraulic characteristics based on pore-size distribution models may need to include factors such as variations of radii along a pore, pore connectivity and tortuosity. These factors can help to provide a more accurate representation of the complex pore geometry in real soils.

2.2. Type 2: Point prediction of the water retention characteristic

Early forms of PTFs are regression equations that predict specific points of interest of mainly the water retention characteristic (Gupta and Larson, 1979; Rawls et al., 1982; Ahuja et al., 1985). Consequently these functions often have the following general form:

$$\theta_h = a^*\text{sand} + b^*\text{silt} + c^*\text{clay} + d^*\text{organic matter} + e^*\text{dry bulk density} + \cdots + x^*\text{variable } X \quad (1)$$

where θ_h is the water content at pressure head h and a, b, c, d, e and x are regression coefficients. Variable X is any other basic soil property that can easily be measured. The coefficients a through x are determined by regression of θ at, for example, $h = -10$ kPa versus relevant soil properties. The advantage of this approach is that fairly accurate predictions can be made for specific points along the water retention curve. Another advantage is that it offers insight in which soil properties are relevant for predicting the water content θ at a specific pressure head h. For example, predicting θ at $h = -1500$ kPa will relate, among other properties, to surface area (e.g. clay) while θ at $h = -10$ kPa will relate to macrostructure (e.g. bulk density). Clear disadvantages are that a large number of regression equations are required to quantify the complete soil moisture retention characteristic and that the output tends to be tabular. The latter format is generally more limited as it may hamper the efficient inclusion of hydraulic characteristics in simulation models.

2.3. Type 3: Prediction of parameters used to describe the complete hydraulic characteristics

Whereas under Type 1 theoretical models are used to predict hydraulic characteristics on the basis of physical principles, under types 2 and 3 regression models are developed. In the latter case no theoretical background is provided but emphasis is on models that give a sufficiently accurate description of, for example, soil hydraulic conductivity. For the latter group of predictive regression models, the term Pedo-Transfer Functions (PTF) has been introduced by Bouma (1989). PTFs are defined as functions that relate different soil characteristics and properties with one another or to land qualities. PTFs are functional relationships that transfer available soil properties (e.g. texture, structure and organic matter content) into missing soil properties (e.g. soil hydraulic and soil chemical characteristics). In contrast to Type 2, PTFs of Type 3 usually predict parameters in models describing the complete θ–h–K relationship. This approach is more straightforward than the point prediction procedure since the results are directly applicable in simulation models. Selection of explanatory variables, decisions on the functional form and the type of error model are usually guided by process understanding.

3. Functions used to describe the water retention characteristic

Soil hydraulic characteristics are often presented as a function rather than as a table. This is because a function can easily be incorporated in simulation models. Several functions exist for the description of water retention and hydraulic conductivity. A number of commonly used equations are briefly described.

Darcy's law states that water flux in porous media equals hydraulic conductivity times gradient of soil water potential. Combination of Darcy's law with the expression for conservation of mass yields Richards (1931) partial differential equation for water flow in unsaturated soil:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left[K(h)\left(\frac{\partial h}{\partial z} - 1\right)\right] \tag{2}$$

where h is the soil water pressure head, θ is the volumetric water content, K is the hydraulic conductivity, t is time and z is soil depth.

To solve this equation, information is needed on the $h(\theta)$ water retention- and $K(h)$ conductivity relationships. For the description of these relationships a wide range of different equations is available (Vereecken, 1992). A power law water retention equation is the Brooks and Corey (1964) equation:

$$S = \left(\frac{h_b}{h}\right)^{\lambda} \tag{3}$$

where S is the saturation degree, $S = (\theta - \theta_r)/(\theta_s - \theta_r)$, θ_s is the maximum water content (defined by various authors as porosity, saturated water content, satiated water content, or water content at air entry) $m^3\,m^{-3}$, θ_r is the residual water content (never defined as a measurable value) $m^3\,m^{-3}$ and h is the pressure head. The air entry pressure head, h_b, and the pore distribution index, λ, are empirical fitting parameters. Eq. (3) with $\theta_r = 0$ is often called Campbell's water retention equation (i.e. Smettem et al., 1999). Anderson et al. (1985) and Gregson et al. (1987) presented the Brooks–Corey Eq. (3) in the form:

$$\log h = a + b \log \theta \tag{4}$$

and found a very close correlation ($R^2 = 0.98$) between parameters a and b.

A water retention equation based on a logistic function was first proposed by Brutsaert (1967) in the form:

$$S = \frac{1}{1 + (\alpha h)^n} \tag{5}$$

where α and n define the shape of the curve; the capillary space appears to be half saturated when $h = 1/\alpha$ and $dS/d(\ln h) = n/4$. This means that the larger n, the steeper the water retention curve at the inflection point. Van Genuchten (1980) suggested the following more flexible equation:

$$S = \frac{1}{[1 + (\alpha h)^n]^m} \tag{6}$$

This equation is used mostly under the assumption of $m = 1 - 1/n$.

Water retention equations based on a probability

integral were proposed by D'Hollander (1979):

$$S = \frac{1}{2}\mathrm{erfc}\left(\frac{1}{\sigma\sqrt{2}}\ln\frac{h}{h_0}\right) \quad (7)$$

where σ is the standard deviation of the lognormal distribution of pore radii, h_0 corresponds to the geometric mean pore radius. Kosugi (1994) modified the derivation of Eq. (7) and arrived at the following equation:

$$S = \frac{1}{2}\mathrm{erfc}\left(\frac{1}{\sigma\sqrt{2}}\ln\frac{h}{h_0} - \frac{\sigma}{\sqrt{2}}\right) \quad (8)$$

Parameters θ_r, h_b, and λ in Eq. (3), θ_r, α, m, and n in Eqs. (5) and (6), σ and h_0 in Eqs. (7) and (8) are empirical fitting parameters. Their values are being predicted by pedotransfer functions, which in turn, are developed from measured data sets. For example, parameters in Eq. (3) were predicted by Ghosh (1976), Clapp and Hornberger (1978), Cosby et al. (1984), Rawls and Brakensiek (1985), Saxton et al. (1986), Smettem et al. (1999) and Mayr and Jarvis (1999). PTFs for the parameters of Eq. (5) were developed by Pachepsky et al. (1982a) and Vereecken et al. (1989).

PTFs for Eq. (6) were built by many authors including Wösten and Van Genuchten (1988), Bachmann and Hartge (1991), Schaap and Bouten (1996), Scheinost et al. (1997), Schaap et al. (1998), Tomasella and Hodnett (1998) and Minasny et al. (1999). PTFs for the parameters of Eq. (7) were developed by Váral-lyay et al. (1982). The accuracy of a number of the listed PTFs is presented and discussed in Section 10.

A separate class of pedotransfer water retention functions is based on the additivity hypothesis, i.e. composing soil water retention from water retention of soil constituents (Gupta et al., 1977; Arya and Paris, 1981; Haverkamp and Parlange, 1986; Serra-Witting et al., 1996; Zeiliguer et al., 2000). The hypothesis is that soil water retention can be approximated by adding up water retention of pore subspaces. These PTFs do not have parameters to fit and seem to work well in sandy soils. In soils with a broader particle size distribution and hierarchical structure, fine material hidden between large particles takes over the space assumed to be reserved for water retention of larger particles. This may be a source of error and therefore the additivity models still need to be tested with a comprehensive database.

4. Functions used to describe the hydraulic conductivity characteristic

Saturated hydraulic conductivity (K_{sat}) is predicted either directly from soil properties or from measured soil water retention. In the latter case, PTF output is not saturated hydraulic conductivity itself, but rather coefficients in the equation relating K_{sat} to water retention. One way to use information on water retention is to apply the modified Kozeny-Carman equation. Ahuja et al. (1984) suggested that a modified Kozeny–Carman equation could be used to predict K_{sat} from effective porosity defined as the difference between the total porosity and water content at −33 kPa pressure head. The proposed relationship was:

$$K_{sat} = B\phi_e^n \quad (9)$$

where ϕ_e is the effective porosity and B and n are shape parameters. In practice, the exponent n is often set to two and the coefficient B is related to the hydraulic radii of flow channels. Ahuja et al. (1984) later considered both B and n to be empirical parameters. Although Eq. (9) fitted data well, its parameters B and n varied considerably from one data set to another (Ahuja et al., 1989; Franzmeier, 1991; Timlin et al., 1996).

A substantial effort was made to predict K_{sat} by using the complete water retention curve and by considering soil pore space as a capillary bundle with various patterns of connectivity and tortuosity. The Kozeny–Carman law was applied to each capillary or to a group of capillaries (Burdine, 1953; Millington and Quirk, 1959; Green and Corey, 1971). Brutsaert (1967), Alexander and Skaggs (1987) and Raats (1992) reviewed a large number of statistical capillary bundle models and reformulated them as closed integral expressions. Snyder (1996) inspected these expressions and found that the majority of them can be represented by a single relationship:

$$K_{unsat} = k_0\theta^L\left\{\int_0^\theta \frac{(\theta - x)^\beta}{[h(x)]^{\frac{2}{\delta}+\gamma}}\,\mathrm{d}x\right\}^\delta \quad (10)$$

where k_0, L, β, γ, and δ are empirical parameters. The capillary bundle models originally were meant to predict K_{sat}. However, it eventually became clear that a matching factor is needed to adjust the

integrated permeability of a capillary bundle to K_{sat}. No unique way of adjustment could be suggested, although various ingenious suggestions have been made (Green and Corey, 1971; Roulier et al., 1972; Gradwell, 1974; Denning et al., 1974; Gardner, 1974; Carvallo et al., 1976; Cameron, 1979). Presently, the main use of Eq. (10) is prediction of unsaturated hydraulic conductivity K_{unsat} as a function of pressure head or water content under the condition that at least one point of the conductivity characteristic is measured.

Empirical parameters in Eq. (10) represent pore space properties that are important for water transport: variations of radii along a pore, pore connectivity and tortuosity. Parameters β and δ account for the effect of pore radii variation along a pore on the hydraulic radius of the pore. The multiplier θ^L accounts for the occurrence of continuous pores (Millington and Quirk, 1959). Mualem and Dagan (1978) interpreted the multiplier θ^L as a tortuosity factor reflecting a decrease in pore effective radii depending on soil saturation. Russo (1988) stressed the need to treat the value of L as an unknown parameter for a given soil. Recently, PTFs were developed to predict L (Vereecken, 1995; Wösten et al., 1995; Wösten et al., 1999). The value of L was found to vary between -10 and 10 (Van Genuchten et al., 1989).

New physical models of soil pore structure have been developed in recent scaling studies to understand and simulate dependencies of hydraulic conductivity on water contents (Sheppard, 1993; Crawford, 1994; Giménez et al., 1997). The resultant equation of these models is:

$$K_{unsat} = \frac{A}{h^B} \tag{11}$$

which is known as Campbell's hydraulic conductivity equation (Campbell, 1974) and can be derived as a special case of Eq. (10). Ahuja and Williams (1991) used Campbell equation for hydraulic conductivity (11) in the form:

$$\log K_{unsat} = a + b \log h \tag{12}$$

and found a good correlation between parameters a and b. This high correlation between parameters can be used in PTF development as, in this case, only one of the parameters in the power law equation needs to be predicted.

Also equations not based on the capillary bundle models were proposed to predict K_{unsat}. In particular, Bhatnagar et al. (1979) observed a linear relationship between log K_{unsat} and water content θ, and suggested to correlate $\mathrm{d}(\log K_{unsat})/\mathrm{d}\theta$ with texture and other soil properties. Lin et al. (1999) entertained a similar idea by introducing the parameter $\alpha_{macro} = \ln(i_0/i_{0.03})/0.03$, where i_0 and $i_{0.03}$ are infiltration rates at 0 and -0.3 kPa pressure head. Clay content and bulk density were the leading α_{macro} PTF inputs. Jaynes and Tyler (1984) proposed to predict parameters in the unsaturated hydraulic conductivity equation as follows:

$$\log K_{unsat} = a_{JT} - b_{JT} h^{1/2} \tag{13}$$

They worked in sandy subsoils and found values of a_{JT} to vary between 1.4 and 2.9 and b_{JT} between 0.57 and 1.5.

5. Grouping data prior to pedotransfer function development

A database of measured soil hydraulic characteristics can be subdivided into groups of more uniform soils. The advantage of this approach is that correlation of hydraulic characteristics with other soil properties is probably more stable and consistent within groups of soils that have similar flow processes. Next, more accurate PTFs can be developed for groups as compared to the database as a whole. Three approaches are pursued with respect to grouping:

- Grouping and calculating average hydraulic characteristics for each group. No PTFs within groups are developed with this approach. The group name/number is the sole PTF input and is actually used as a nominal explanatory variable.
- Grouping and developing PTFs separately for each group using various different soil properties.
- No grouping at all and developing PTF equations for all data sets.

Wösten et al. (1990a) called PTFs based on a preliminary grouping 'class' PTFs whereas they used the term 'continuous' PTFs to denote PTFs that are developed without grouping. Different grouping criteria are used. Franzmeier (1991) showed that

grouping soils by genetic horizons and parent material is preferable to grouping by texture in determining gravimetric water contents at −33 and −1500 kPa. Also De Jong and Loebel (1982), Bruand (1990) and Pachepsky et al. (1982a, 1996) grouped soils using genetic classification. Wösten et al. (1990a) grouped soils based on an assessment of the functional behavior of different horizons. If for instance, the simulated evaporation deficit or the simulated flux at a certain depth is similar for two different soil horizons then these horizons are grouped together. The advantage of testing on functional behavior is that not the hydraulic characteristics themselves are compared but rather the effects these characteristics have on practical aspects. The importance of texture is such that several attempts were made to predict hydraulic characteristics for different textural classes. The Soil Survey Staff textural classes were used by Clapp and Hornberger (1978) and McCuen et al. (1981) to predict parameters in the Brooks–Corey equation for water retention. Clapp and Hornberger (1978), McCuen et al. (1981), Rawls et al. (1982) and Gumps (1974) suggested using soil textural class as a sole predictor of K_{sat}. Later, Rawls et al. (1998) accumulated and analyzed the US national database of about 1000 data sets on K_{sat} values. The data were grouped by texture and then into two porosity classes. There was a general decline both in variation and in median value as the average clay content in samples of the group increased. High porosity samples had higher hydraulic conductivity but the difference became negligible as the clay content increased. Cosby et al. (1984) found it sufficient to distinguish four broad textural classes obtained by aggregating Soil Survey Staff classes. Krahmer et al. (1995) presented hydraulic characteristics for 31 textural classes. Wösten et al. (1999) developed PTFs for FAO texture classes in combination with the distinction between topsoil and subsoil using the HYPRES database. Williams et al. (1992) and Danalatos et al. (1994) suggested distinguishing weakly structured and well structured soil horizons. A grouping by mineralogy and genesis before developing PTFs was suggested by Puckett et al. (1985). Hartge (1969) and Bachmann and Hartge (1991) suggested using similarity in particle size distributions instead of texture classes to group soils. McKenzie and Jacquier (1997) suggested to use field texture class as a primary grouping criterion, and then to apply various field-morphology based grouping criteria for further dichotomic subdivisions of data in ever-smaller subgroups.

Interest in using landscape position as a grouping criterion is growing as studies show that landscape position may account for a substantial part of the variation. The reason for this is that soils and thus also the associated soil properties, vary with landscape position. As such landscape position is considered to be an integrator of different soil properties. Bathke and Cassel (1991) found significant differences in predictions of K_{sat} using separately developed PTFs for the same soil series in different landscape positions (interfluve, shoulder, linear slope and footslope).

6. Soil properties used as input parameters in pedotransfer functions

Soil properties affecting water retention and transport of water and chemicals in soils are manifold. Table 1 lists the properties used most often because of their availability or because they proved to be the most promising ones. This section is restricted to soil properties used for the prediction of the hydraulic characteristics. In Section 9, soil properties are discussed used for prediction of other soil characteristics. The role of the different soil properties as predictors in PTFs is reviewed briefly.

Particle size distribution is used in almost any pedotransfer function. Different national and international classification systems use often quite different particle size classes. As a consequence, textural classes used in PTFs vary considerably. However, using sand, silt and clay contents is a common approach (i.e. MacLean and Yager, 1972; Pachepsky et al., 1982a; Rajkai and Várallyay, 1992; Williams et al., 1992; Shein et al., 1995; Wösten et al., 1999). To characterize particle size distributions, the median diameter was found useful in soils with wide texture ranges (Bloemen, 1980; Campbell, 1985). Minasny et al. (1999) and Scheinost et al. (1997) used the median diameter along with the geometric standard deviation to predict soil water retention. Mishra et al. (1989) did the same to predict K_{sat}. To use the particle size distributions, it is desirable to have functions suitable to

Table 1
Soil properties often used in pedotransfer functions

Particle size properties	Hydraulic characteristics	Morphological properties	Chemical/ mineralogical properties	Mechanical properties
Sand, Silt, Clay	Water content at	Bulk density	Organic carbon	Penetration
Fine sand	− 33 kPa	Porosity	Organic matter	Resistance
Very coarse sand, coarse fragments	− 1500 kPa	Horizon	CEC	
		Structure	Clay type	
Median or Geometric mean particle size	Reference moisture retention curve	grade	$CaCO_3$	
		size	Iron	
		shape		
Water-stable aggregates		Colour		
		Consistence		
		Pedality		

approximate the whole distribution or to approximate the particle size distribution within a large diameter range. This is needed when the textural particle size distribution is characterized by a limited number of fractions (Zeiliguer et al., 2000), or when data come from different sources with different fraction diameter ranges (Nemes et al., 1999).

Texture alone was reported to be a good predictor of saturated hydraulic conductivity in sandy soils (Jaynes and Tyler, 1984; El-Kadi, 1985b). Clay content was a leading texture parameter to be correlated with K_{sat} in databases comprising of soils other than sandy soils (Puckett et al., 1985). It is good to remember that particle size distribution or texture itself is probably a poor predictor of for instance K_{sat}. Most likely the associated but difficult to quantify soil structure is the determining soil property in predicting soil hydraulic characteristics.

Porosity or bulk density was an important variable in PTFs developed by Rawls et al. (1982, 1983), Aina and Periaswamy (1985), Rajkai and Várallyay (1992), Bruand et al. (1996) and Wösten et al. (1999).

Limited water retention data at, for instance, two points on the water retention curve considerably improved predictions of water retention in the work of Ahuja et al. (1985), De Jong (1983), Rawls et al. (1982) and Paydar and Cresswell (1996).

Mineralogical properties such as the proportion of montmorillonite or illite clay were shown by Ali and Biswas (1968) to have little effect on water retention (about 9%) at −1500 kPa but amounts to 240% at −10 kPa pressure head. Baumer and Brasher (1982) suggested the mineralogical composition as a primary grouping criteria to predict soil water retention.

Organic matter/carbon content was successfully used by Rawls et al. (1982, 1983) and Wösten et al. (1999) as PTF input. Bloemen (1980) demonstrated a correlation between bulk density and organic matter content in his data sets and indicated that bulk density effectively substituted organic matter content.

Chemical properties such as content of iron oxides were dominating properties to affect soil water retention. Rajkai and Várallyay (1992) found the $CaCO_3$ content to be the second most important PTF input to predict water retention at −1500 kPa.

Landscape position was suggested to be used by Rhodenburg et al. (1986) and Bork (1988) as a topographic variable in pedotransfer functions along with basic soil properties. Pachepsky et al. (2001a) showed a good relationship of water retention with slope and curvature of soil surface computed over a 30×30 m grid.

Mechanical properties and shrink–swell parameters as characterized by the coefficient of linear extensibility (COLE) was used to predict both water retention (Baumer, 1992; Pachepsky et al., 1998) and K_{sat} (McKenzie et al., 1991).

Soil structure and morphology descriptors are generally beneficial to pedotransfer function development. Williams et al. (1992) included the field attribute pedality in water retention PTFs. A detailed count of lengths and widths of voids allowed

Anderson and Bouma (1973) to compute hydraulic conductivity of an argillic horizon of silt loam soil using a Kozeny–Carman equation for flow in slits.

Soil management in the form of no-till resulted in an observed soil water retention to be 0.03–0.12 $m^3 m^{-3}$ larger than in conventionally tilled soil in the range of capillary pressures from −30 to −400 kPa (Azooz et al., 1996). Comparison of pre- and post tillage shapes of water retention curves appears to be indicative for changes in hydraulic characteristics (Klute, 1982). If tillage operations produce an increase in bulk density of a soil with an unimodal particle size distribution, then K_{sat} will decrease $2-5$ times. If on the other hand, tillage operations create a bimodal particle size distribution in a soil with an essentially unimodal distribution, it is expected that both K_{sat} and water retention close to saturation will increase.

Hierarchical methodologies to predict soil parameters can be a solution, in case requested input parameters for PTFs are not available. Several strategies were applied to counter the absence of input parameters. Baumer et al. (1994) proposed to use the same PTF and predict its requested input parameters in different ways depending on available information. Contrarily, Schaap et al. (1998) proposed to develop and use different PTFs for different levels of detail of input parameters. Batjes (1996) developed a system of hierarchical rules to predict available water for main soil series of the FAO–UNESCO world soil map. He proposed not to try to predict PTF input parameters, but to extrapolate PTF outputs from well known to less known soil series.

7. Methods to develop pedotransfer functions

When the set of PTF input parameters is defined and the PTF output is decided upon, a method has to be selected to build the relationship relating input and output. Techniques used for PTF development are regression analysis, neural networks, group method of data handling and Classification and Regression Trees (CART). These different techniques are briefly described. It is fair to say that the success of any technique will largely depend on the quality and appropriateness of the original measurements stored in the databases. For instance, a great deal of standard soil morphological description is of little value because of operator dependency and because of the complex link between this parameter and hydraulic characteristics.

7.1. Regression analysis

In the beginning PTFs were built using almost exclusively linear regressions (i.e. Gupta and Larson, 1979). Nonlinear regressions gradually replaced linear regressions (Rawls and Brakensiek, 1985). An advantage of regression techniques is that most essential input parameters can be found automatically using stepwise regression. A drawback of regressions is that any equation is able to mimic only a particular shape of the dependence. Another drawback of regressions became apparent in the early nineties when large databases containing digitized soil hydraulic characteristics became available. The number of soil properties available as PTF inputs became very large and the type (shape) of dependence on all of them (or some of them) was almost impossible to establish. One remedial approach is to use principal component analysis to find a small number of new parameters that are linear combinations of the original inputs and can explain a large percentage of variability within samples (Lin et al., 1999). Many other research and engineering fields encountered similar problems in dealing with large numbers of input parameters with unknown dependencies between input and output. Information technologies responded with data mining tools that allowed the discovery of dependencies between parameters in databases without assumptions on the type (shape) of the dependencies and without an *apriori* list of parameters that needs to be included in a relationship.

7.2. Artificial neural networks

Artificial neural networks (ANNs) are becoming a common tool for modelling complex 'input–output' dependencies (Maren et al., 1990; McCord and Illingworth, 1990). The advantage of ANNs is their ability to mimic the behavior of complex systems by varying the strength of influence of network components on each other as well as its range of choices of structures of interconnections among components. After establishing the network structure and finding

coefficients to express the degree of influence of the network components on each other, an ANN becomes a special type, complex formula relating input with output values. This formula can be used like a regression formula. An ANN consists of many interconnected simple computational elements called nodes or neurons. It should be stressed that there are many types of neurons, many types of connections between them, and, therefore, many types of possible neural networks (Hecht-Nielsen, 1990). One type of ANN, namely feed-forward ANN, was almost exclusively used to build PTFs (Pachepsky et al., 1996; Schaap and Bouten, 1996; Schaap et al., 1998; Koekkoek and Bootlink, 1999; Minasny et al., 1999). The ANN used by Tamari et al. (1996) for prediction of K_{sat} represents an exception. These authors applied neural networks using a radial based function. A diagram of a multilayer feed-forward ANN is given in Fig. 1. Outputs of neurons are used as inputs to other neurons in the network as shown in Fig. 1. The data flow in this figure goes from the input layer through the hidden layer to the output layer. The network is called feed-forward because it does not have any feedbacks or parallel connections within a layer of neurons. A network may have more than one hidden layer. The manner in which ANNs approximate functions can be regarded as a generalization of regression analysis. When the number of inputs is larger than three, ANNs usually do better than regression techniques even if the latter use nonlinear functions of input data, i.e. as in polynomial regression (Hecht-Nielsen, 1990).

7.3. Group method of data handling

The group method of data handling (GMDH) has unlike ANNs, a built-in algorithm to retain only essential input variables in a flexible net of regression equations, to relate inputs to outputs (Pachepsky et al., 1998). Group method of data handling is a technique of finding an approximate relationship between a set of input variables $x_1, x_2, \ldots, x_N$ and an output variable y (Farlow, 1984). When the number of input variables is very large, or when the relationship between inputs and output is very complex, GMDH successfully competes with statistical regression (Hecht-Nielsen, 1990).

7.4. Classification and regression trees

Classification and Regression Trees (CART) are

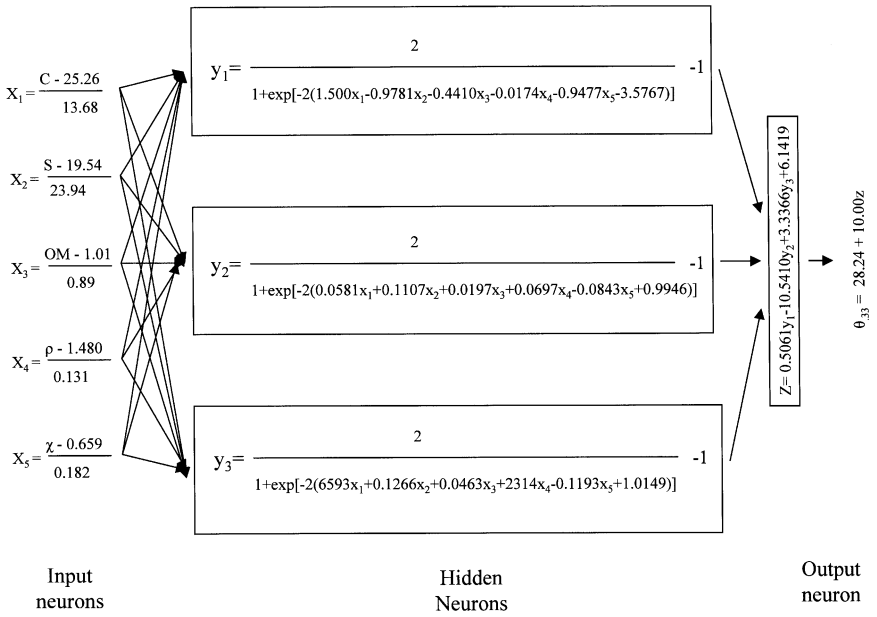

Fig. 1. Example of a feed-forward ANN to predict water content at −33 kPa from clay C, sand S and organic matter OM contents (%), bulk density ρ (g cm^{-3}), and clay activity ratio χ, defined as a ratio of the cation exchange capacity of soil mineral fraction to the clay content in soil. The network has five linear input level neurons, three hidden layer networks, and one linear output layer neuron.

recursive data partitioning algorithms (Breiman et al., 1984) that initially split data sets into two subsets based on the predictor variable that minimizes the variance in the response. It then does the same on each of the subsets and so on recursively. The output is a tree with branches and terminal nodes. The predicted value at each terminal node is the average at that node. CARTs are best suited to very large data sets where the data are nominal or on coarse steps. There is a hierarchical structure to the data and binary splits are appropriate. Using CART to develop PTFs was pioneered by McKenzie and Jacquier (1997).

Fig. 2 shows the accuracy of predicting water content at −33 kPa pressure head with the last three methods: (a) backpropagation artificial network, (b) group method of data handling, (c) classification and regression trees. As can be seen, the accuracy of the three methods is quite comparable. In all three cases the root-mean square error is around 3.4 vol.%, the R^2 value of the regression is around 0.9, the slope of the regression is close to 1 and the intercept is about 0.001 vol.%. The fact that these methods yield comparable results indicates also that major progress has not to be expected from new statistical methods but rather from better data.

8. HYPRES as a practical example of the use of a database to develop pedotransfer functions

For the development of PTFs large, good quality data sets are required comprising measured hydraulic characteristics of a wide variety of soils. An example of such a large data set is the database of HYdraulic PRoperties of European Soils (HYPRES). The HYPRES database contains information on a total of 5521 soil horizons (Wösten et al., 1999). Of these, 4030 horizons had sufficient soil hydraulic data that could be used for the development of PTFs. The soil information is donated by 20 institutions from 12 European countries. Problems in constructing this large international database were twofold; (i) various countries use different soil classification systems with the consequence that soil texture classes have different meanings in different countries, and (ii) due to the application of different measurement techniques the number of measured individual points along the various hydraulic characteristics varies considerably. Both problems had to be resolved to arrive at an international database that holds compatible, good quality national data. In this case it was decided to adhere to the Food and Agriculture Organisation (FAO) (1990) and the Soil Survey Staff (1951) particle-size class intervals. As a consequence, a new interpolation technique had to be developed to get an accurate prediction of missing particle size fractions (Nemes et al., 1999). In turn, this interpolation technique was used to arrive at a standardized database. Even more important, use of different measurement techniques by the different institutions resulted in a marked imbalance in the number of measured soil hydraulic data pairs for the different soil horizons. To avoid statistical bias, this imbalance was eliminated by parameterizing the individual hydraulic characteristics with Eqs. (6) and (10) according to Van Genuchten et al. (1991). As a result

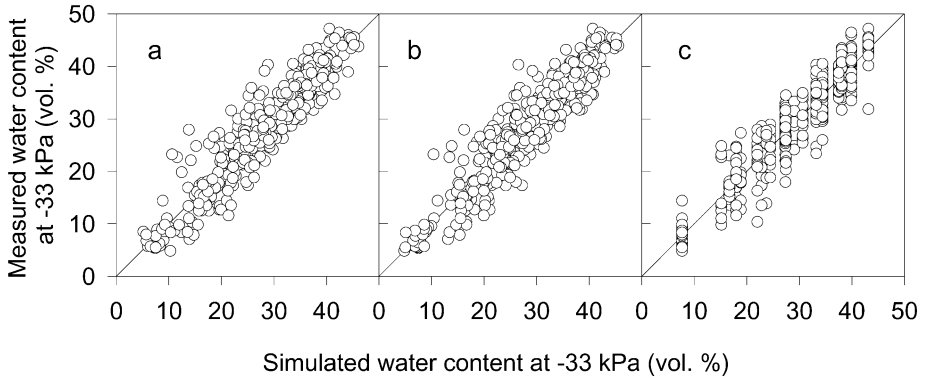

Fig. 2. One-to-one diagrams showing accuracy of predicting water content at −33 kPa pressure head with three methods, (a) backpropagation artificial neural network, (b) group method of data handling, (c) classification and regression trees.

the measured hydraulic characteristics became available as a compatible set of optimised model parameters (i.e. θ_r, θ_s, K_{sat}, α, L and n).

Pedotransfer functions for the different texture classes were derived by firstly using the optimised parameters to determine the moisture contents and conductivities at 14 arbitrarily pressure heads. As the $\theta(h)$ and $K(h)$ relationships are lognormally distributed, the geometric mean moisture contents and conductivities at the 14 pressure heads were calculated. In addition to the geometric mean values, the θ and K values within one standard deviation were also calculated. These standard deviations give an indication of the degree of variation of the individual curves around the geometric mean curve. Next the geometric mean values at the 14 pressure heads were again fitted with Eqs. (6) and (10) to arrive at optimised model parameters for the mean characteristics. Since these parameters represent the mean hydraulic characteristics for a soil texture class they are called class pedotransfer functions. In total, class pedotransfer functions for 11 texture classes have been established. The 11 texture classes consist of 5 FAO texture classes, subdivided in topsoil and subsoil texture classes, plus the FAO texture class organic soils used to prepare the European soil map on a scale 1:1 000 000. Fig. 3 shows the calculated geometric mean water retention and hydraulic conductivity characteristic and the standard deviations for the texture class 'Medium Fine Topsoils'.

In addition to the development of class pedotransfer functions, linear regression was used to investigate the dependency of each model parameter on more easily measured, basic soil properties. To comply with a number of physical boundary conditions, transformed parameters rather than the original model parameters were used in the regression analysis. In this case, the imposed boundary conditions were: $K_{sat} > 0$, $a > 0$, $n > 1$ and $-10 < L < +10$. The following basic soil properties were used as regressed variables: percentage clay, percentage silt, percentage organic matter; bulk density and also the qualitative variable topsoil or subsoil. Linear, reciprocal, and exponential relationships of these basic soil properties were used in the regression analysis, and possible interactions were also investigated. As a consequence, the resulting regression model consists of various basic soil properties and their interactions, all of which contribute significantly to the description of the transformed model parameters. The models were selected using a subset selection method. Since these pedotransfer functions require point specific soil data instead of class average texture data, they are called continuous pedotransfer functions (Vereecken, 1992; Tietje and

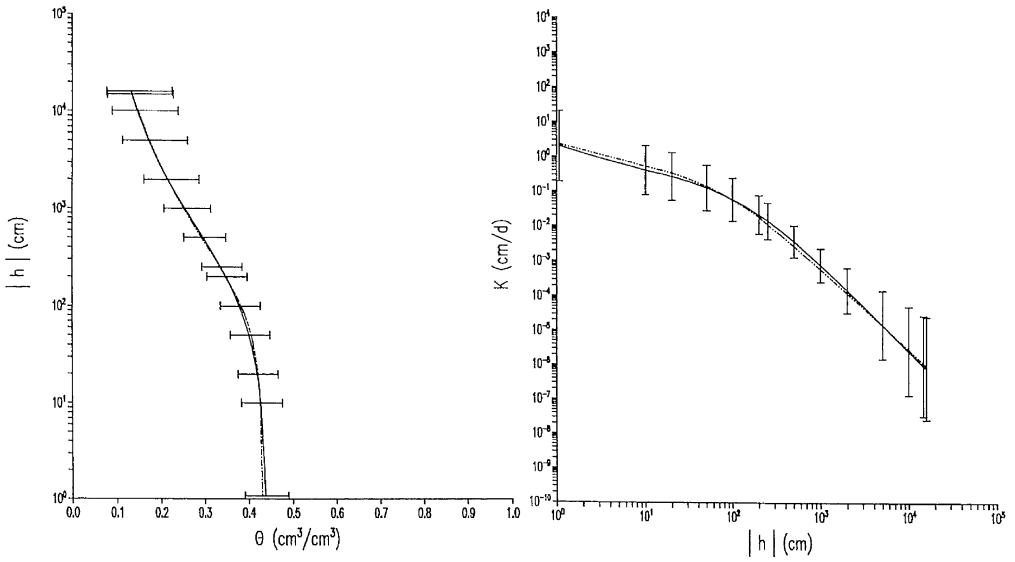

Fig. 3. Geometric mean water retention (left graph) and hydraulic conductivity (right graph) characteristic (solid lines), standard deviations (bars) and Mualem–van Genuchten fits (dotted lines) for the texture class 'Medium Fine Topsoil' (after Wösten et al., 1999).

Tapkenhinrichs, 1993). The continuous pedotransfer functions developed using the HYPRES database are presented in Table 2.

While class pedotransfer functions predict the hydraulic characteristics for rather broadly defined soil texture classes, and therefore do not provide site specific information, continuous pedotransfer functions can be applied in case of more site specific applications. The R^2 values obtained indicate that the predictions of the hydraulic characteristics when using continuous pedotransfer functions are fairly inaccurate. Subdividing the complete dataset in subsets of similar soil texture might improve these predictions.

The class pedotransfer functions for the 11 FAO texture classes are used to translate the representative profiles for the mapping units of the European soil map at a scale of 1:1 000 000 into soil hydraulic profiles. The result is a transformed European soil map that gives a spatial picture of the soil hydraulic composition of the unsaturated zone of European soils. Based on this map it was possible to prepare a map showing total available water on a European scale. This map is just one example of the type of new spatial information that can be generated when pedotransfer functions are used in combination with other existing spatial soil data. Other possible new products could be a travel time map for solutes or an infiltration rate map for erosion studies.

The HYPRES study showed that it is possible to assign soil hydraulic characteristics to soils with a textural composition comparable to the soils for which the pedotransfer functions have been derived. However, care should be taken to use the functions for prediction of hydraulic characteristics of soils outside the range of the original database. Class pedotransfer functions give the mean hydraulic characteristics for rather broadly defined soil texture classes. As a consequence, these functions are generally better applicable, however, they give limited site-specific information. In contrast, continuous pedotransfer functions are more site-specific, but their general applicability is limited, as they require more specific input data.

An example of an interregional comparison of PTFs is given in Fig. 4 where 21 different PTFs are applied to predict water contents at −33 and −1500 kPa. Table 3 gives the details of the 21 PTFs tested. The test is performed against a measured dataset from Oklahoma. Fig. 4 illustrates various difficulties encountered in PTF reliability predictions. PTF #1 has the CEC of clay fraction as an essential input. An average value of the CEC/clay ratio = 0.5 was applied to all data to compute the data in Fig. 4.1. PTF # 5 is derived from data on only 6 soils and it fails when tested with a large database. Similarly PTF # 7 is derived from data on only 43 soils. PTF # 6 for the field capacity was developed with actual field data and an attempt to equate the field capacity to the water content at −33 kPa is unsuccessful. PTFs # 2 and # 8 were derived for a clay mineralogy that is distinctly different from the one in Oklahoma. They tend to overestimate water retention at −1500 kPa. For the same reason PTF # 9, PTF # 13, and PTF # 19 tend to underestimate it. PTFs # 3 and 18 are developed for tropical soils and, therefore, do not give satisfactory predictions of field capacity. However, these PTFs

Table 2
Continuous pedotransfer functions developed from the HYPRES database (θ_s is a model parameter, α^*, n^*, l^* and k_s^* are transformed model parametes in the Mualem–van Genuchten equations; C = percentage clay (i.e. percentage < μm); S = percentage silt (i.e. percentage between 2 μm and 50 μm); OM = percentage organic matter; D = bulk density; topsoil and subsoil are qualitative variables having the value of 1 or 0 and ln = natural logarithm)

$$\theta_s = 0.7919 + 0.001691 \times C - 0.29619 \times D - 0.000001491 \times S^2 + 0.0000821 \times \mathrm{OM}^2 + 0.02427 \times C^{-1} + 0.01113 \times S^{-1} + 0.01472 \times \ln(S) - 0.0000733 \times \mathrm{OM} \times C - 0.000619 \times D \times C - 0.001183 \times D \times \mathrm{OM} - 0.0001664 \times \mathrm{topsoil} \times S \quad (R^2 = 76\%)$$

$$\alpha^* = -14.96 + 0.03135 \times C + 0.0351 \times S + 0.646 \times \mathrm{OM} + 15.29 \times D - 0.192 \times \mathrm{topsoil} - 4.671 \times D^2 - 0.000781 \times C^2 - 0.00687 \times \mathrm{OM}^2 + 0.449 \times \mathrm{OM}^{-1} + 0.0663 \times \ln(S) + 0.1482 \times \ln(\mathrm{OM}) - 0.4546 \times D \times S - 0.4852 \times D \times \mathrm{OM} + 0.00673 \times \mathrm{topsoil} \times C \quad (R^2 = 20\%)$$

$$n^* = -25.23 - 0.02195 \times C + 0.0074 \times S - 0.1940 \times \mathrm{OM} + 45.5 \times D - 7.24 \times D^2 + 0.0003658 \times C^2 + 0.002885 \times \mathrm{OM}^2 - 12.81 \times D^{-1} - 0.1524 \times S^{-1} - 0.01958 \times \mathrm{OM}^{-1} - 02876 \times \ln(S) - 0.0709 \times \ln(\mathrm{OM}) - 44.6 \times \ln(D) - 0.02264 \times D \times C + 0.0896 \times D \times \mathrm{OM} + 0.00718 \times \mathrm{topsoil} \times C \quad (R^2 = 54\%)$$

$$l^* = 0.0202 + 0.0006193 \times C^2 - 0.001136 \times \mathrm{OM}^2 - 0.2316 \times \ln(\mathrm{OM}) - 0.03544 \times D \times C + 0.00283 \times D \times S + 0.0488 \times D \times \mathrm{OM} \quad (R^2 = 12\%)$$

$$k_s^* = 7.755 + 0.0352 \times S + 0.93 \times \mathrm{topsoil} - 0.967 \times D^2 - 0.000484 \times C^2 - 0.000322 \times S^2 + 0.001 \times S^{-1} - 0.0748 \times \mathrm{OM}^{-1} - 0.643 \times \ln(S) - 0.01398 \times D \times C - 0.1673 \times D \times \mathrm{OM} + 0.2986 \times \mathrm{topsoil} \times C - 0.03305 \times \mathrm{topsoil} \times S \quad (R^2 = 19\%)$$

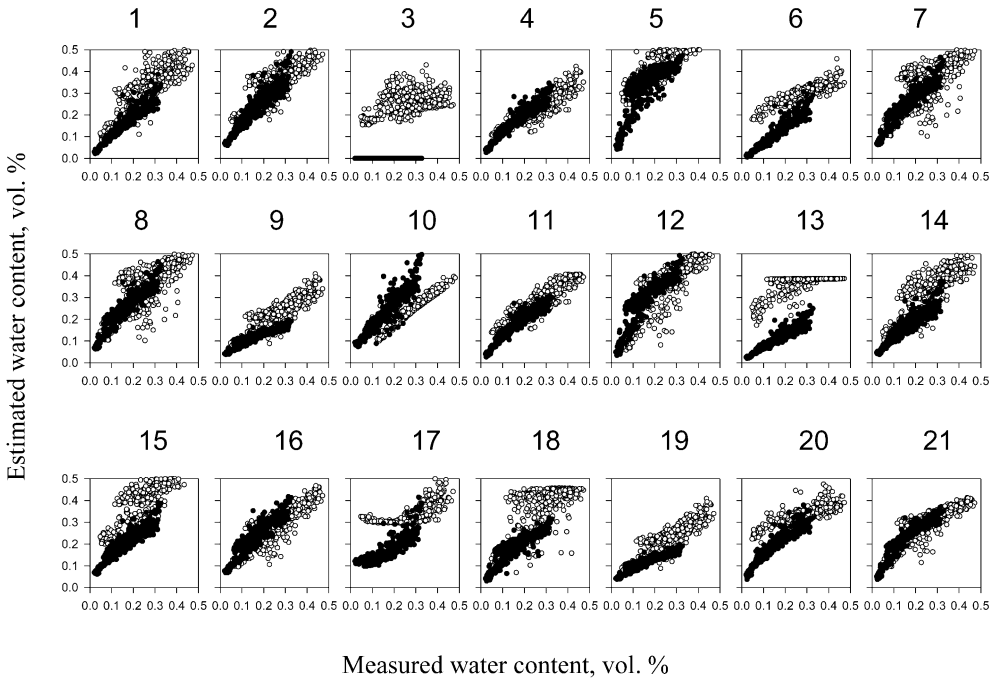

Fig. 4. Water contents at −33 kPa (○) and at −1500 kPa (●) predicted with 21 PTFs developed in various regions of the world and tested against a measured dataset for Oklahoma. Table 3 gives the details of the tested PTFs.

seem to perform well at −1500 kPa. Using only texture leads to unsatisfactory results at low water contents as shown by PTF # 17. PTFs # 11 and # 16 perform best on this test set. The comparison illustrates that, however, some PTFs are more generally applicable than others, quality assessment of PTFs has to be carried out using independently measured soil hydraulic characteristics for soil horizons that fall in the same texture range as the horizons for which the PTFs have been developed.

9. Pedotransfer functions for other soil characteristics

So far this discussion on pedotransfer functions has been focused on the transfer of easy to obtain soil survey information into soil hydraulic characteristics. However, the same soil survey data can be used to make predictions for other soil characteristics as will be demonstrated in this section.

The most common example of an effective parameter is the available soil water capacity in models where soil is represented as a 'bucket' with water contents varying between field capacity and wilting point. To avoid misunderstanding, a strict definition of the terms field capacity and wilting point is always required. Haise et al. (1955) compared field capacity with the water content at −33 kPa (w_{33}) and found a high correlation as well as a significant difference between regression slope and one. Field capacity was substantially higher than w_{33} in coarse-texture soils and substantially lower than w_{33} in fine-texture soils. A similar difference between regression slope and one was demonstrated for wilting point and water content at −1500 kPa. Similar results were observed by Cavazza et al. (1973) who found that average values of field capacity were close to water contents at −20 kPa in loamy soils. However, the regression of water contents at −20 kPa vs water contents at field capacity produced slopes significantly less than one. Rivers and Shipp (1972) and Bennet and Entz (1989) compared field water contents at field capacity with water contents at −10 kPa for coarse-texture soils and observed differences up to 100%. Part of this discrepancy may be attributed to the fact that water content

Table 3
Pedotranfer functions tested for their reliability against a measured dataset for Oklahoma

PTF	Source	Region	Number of samples	Input variables					Comment
				Sand	Silt	Clay	BD	OM	
1	Baumer, 1992	All USA	18 000	+	−	+	+	+	Simplified to remove dependence of CEC
2	Beke and McCormic, 1985	Nova Scotia, Canada	25	+	+	+	+	+	PTF developed for subsoil
3	Bell, 1993	Mexico, ~20°N	148	+	−	−	−	+	
4	Bruand et al., 1994	Central France	20	−	−	+	−	−	
5	Campbell and Shiozawa, 1992	No particular	6	+	−	+	+	−	
6	Canarache, 1993	Romania, mostly mollisols	Unknown	+	+	+	+	+	The field capacity value is measured in the field
7	Gupta and Larson, 1979	Central USA, 10 solid and 33 sediments	43	+	+	+	+	−	
8	Hall et al., 1977	UK, England and Wales	261	+	−	+	−	−	
9	Oosterveld and Chang, 1980	Canada, Alberta	298	+	−	+	+	−	
10	Pachepsky et al., 1982b	Hungary, mostly haplaborols and aquicustolls	230	+	+	+	+	−	Simplified to remove the dependence on depth
11	Petersen et al., 1968	Pennsylvania,	1267	−	−	+	−	−	Did not use separate equations for textural classes
12	Puckett et al., 1985	USA, Lower Coastal Plains	42	+	−	+	+	−	
13	Rajkai and Várallyay, 1992	Hungary, mostly haplaborols and aquicustolls	270	+	−	+	+	+	Is not reliable for higher suctions
14	Rawls et al., 1982	USA, nationwide	5320	+	+	+	−	+	
15	Rawls et al., 1983	USA, nationwide	5320	+	+	+	+	−	
16	Rawls and Brakensiek, 1985	USA, nationwide	5320	+	−	+	+	−	
17	Saxton et al., 1986	USA, nationwide	5320	+	−	+	−	−	
18	Tomasella and Hodnett, 1998	Brazilian Amazoni	614	−	+	+	−	−	
19	Vereecken et al., 1989	Belgium	182	+	−	+	+	+	
20	Williams et al., 1992	Australia	196	+	−	+	−	+	Simplified by setting coarse sand = 0
21	Williams et al., 1992	Australia	196	+	−	+	+	−	Simplified by setting coarse sand + fine sand = sand and assuming soil being pedal

at field capacity is defined differently by various authors. Therefore, to predict the available water content for 'bucket' models, one has to correct values of the available water capacity predicted as the difference between w_{33} and w_{1500} or between w_{10} and w_{1500}. Canarache (1993) and Bell and van Keulen (1995) indicated that soil organic matter content is an important factor in predicting water content in soil at field capacity. Care has to be taken to correctly understand how authors of a model define field capacity since this is often associated with a specific pressure head, i.e, with −10 kPa (Da Silva et al., 1994), −5 kPa (Hollis et al., 1977; MacLean and Yager, 1972).

Predicting bulk density with PTFs is not desirable because direct measurement is relatively cheap and simple. Nevertheless, a substantial number of PTFs have been developed for this purpose. Baumer (1992) used data on texture, organic matter content, and CEC to develop a PTF to relate bulk density to water contents. Kern (1995) analyzed data of about 30 000 soil horizons and found a close correlation between oven dry and −33 kPa bulk density. Manrique et al. (1990) predicted bulk density at −33 kPa from clay and organic matter content. They found that preliminary genetic grouping by suborders greatly improved the accuracy of PTFs, and that different basic properties were needed to predict bulk density at −33 kPa in different soil orders. Rawls (1983) used soil texture and organic matter to predict bulk density.

Sometimes models use lumped hydraulic parameters that are model-specific. Examples are abundant in parameterizations of soil-vegetation-atmosphere interactions (e.g. 'effective soil resistance to water transfer in the liquid phase' (Bastiaanssen, 1991).

Bakker et al. (1987) presented PTFs for predicting oxygen diffusion coefficients in soils (D_s), in $m^2\ s^{-1}$ at 20°C, using the volume fraction of gas (V_g) in soils as input parameter.

Pedotransfer functions also have been developed for soil chemical characteristics. Predictions of CEC and the sum of exchangeable bases were made using clay content, soil organic matter content and pH as input variables (Breeuwsma et al., 1986; Manrique et al., 1990; Bell and van Keulen, 1995; Oberthür et al., 1996). Since CEC can be measured relatively cheap and simple, direct measurement is preferred over predictions with PTFs. Pedotransfer functions for the characterization of the soil phosphorus regime were developed using oxalate extractable aluminum and iron concentrations (Brus et al., 1992). Scheinost and Schwertmann (1995) used clay, dithionite-extractable iron and pH to predict adsorption capacity parameters for isotherms of phosphate adsorption–desorption. Distribution coefficients of heavy metals among liquid and solid phases were predicted with a pedotransfer function using pH, clay and organic matter contents, and CEC as inputs (Bril, 1995). In soil fertility studies, Janssen et al. (1990) established PTFs to predict the potential supply of soil nitrogen, phosphorus and potassium for maize.

Soil mechanical characteristics were predicted from various basic soil properties. Plasticity index and optimum moisture content correlated with clay content and CEC (De la Rosa, 1979; Kay et al., 1997), or with silt content and CEC (Aragón et al., 2000).

Development of PTFs responds to the need of modellers to acquire in a relatively simple and cheap way, good quality input data for their models. Most likely more characteristics will be predicted using PTFs as the models in which the characteristics are used, apply to regional, agricultural and environmental estimates. In any case it is important to make sure that the accuracy of the predictions obtained with PTFs is in accordance with the desired accuracy of the study in which the predictions are going to be used.

10. Accuracy and reliability of pedotransfer functions

As predictive equations, PTFs are routinely evaluated in terms of correspondence between measured and predicted values. When measured values are those used to develop the equation, the accuracy of the equation is evaluated. When measured values are different from the ones used to develop the equation, the reliability is evaluated.

The same statistics are used to evaluate both accuracy and reliability. A multitude of statistics is used in PTF development. The most common ones are listed below, here y_i denotes the actual value, $\hat{y}_i$ — the predicted value, and $\bar{y}_i$ — the average of the actual value y, N is the total number

of observations:

(a) the Spearman correlation coefficient,
(b) the multiple determination coefficient,

$$R^2 = 1 - \frac{\sum_1^N (y_i - \hat{y}_i)^2}{\sum_1^N (y_i - \bar{y}_i)^2}$$

(c) root mean square error RMSE (also called root mean squared deviation RMSD or root mean square residual RSMR)

$$\mathrm{RMSE} = \sqrt{\frac{\sum_1^N (y_i - \hat{y}_i)^2}{N}}$$

(d) mean error

$$\mathrm{ME} = \frac{\sum_1^N (y_i - \hat{y}_i)}{N}$$

(e) the integral mean error and the integral root mean square error (i.e. Tietje and Tapkenhinrichs, 1993):

$$\mathrm{IME} = \frac{1}{b-a}\int_a^b (y - \hat{y})\mathrm{d}y;$$

$$\mathrm{IRMSE} = \sqrt{\frac{1}{b-a}\int_a^b (y - \hat{y})^2 \mathrm{d}y}$$

(f) mean absolute error:

$$\mathrm{ME} = \frac{\sum_1^N |y_i - \hat{y}_i|}{N}$$

(g) t-statistic to test the null hypothesis on the equality to one of the slope in the one-to-one diagram of predicted versus measured values.
(h) t-statistic to test the null hypothesis on the equality to zero of the intercept in the one-to-one diagram of predicted versus measured values.
(i) t-statistic to test the null hypothesis about the equality of means of predicted versus measured values.
(j) F-statistic to test the null hypothesis about the equality of variances of predicted versus measured values.

Some statistics are not reported as measures of accuracy but their critical values are used in PTF development to prevent excessive complexity of PTFs. Those are the Akaike Information Criterion (Russo, 1988), Baron's test (Pachepsky and Rawls, 1999), and F-test to terminate stepwise regression (i.e. Tomasella and Hodnett, 1998; Shein et al., 1995; Wösten et al., 1999).

Studies have been conducted on the ability of PTFs to predict the spatial structure of water retention. Also, parameters of semivariograms have been compared for measured water retention versus water retention predicted with PTFs. For example, Springer and Cundy (1987) did not find significant differences in average measured and PTF predicted hydraulic conductivity and sorptivity. Semivariograms of measured and PTF predicted characteristics were similar in their study. Similarly, Romano and Santini (1997) found that the structure of spatial variability was adequately described when using PTFs for determining soil water retention characteristics. Sinowski et al. (1997) and Heuvelink and Pebesma (1999) reported that in variable landscapes, spatial interpolation of PTF inputs and subsequent application of PTFs provided better results than point-predicting water retention with PTFs and subsequent interpolation of parameters in water retention equations.

10.1. Accuracy of pedotransfer functions

Using the same statistics, accuracy of existing PTFs varies appreciably. Table 4 presents a sample from literature that gives typical values of root-mean square errors achieved with PTFs to predict soil water retention. The RMSE of volumetric water contents ranges from 0.02 to 0.11 $m^3\,m^{-3}$. The smallest RMSE values of 0.02 $m^3\,m^{-3}$, are obtained in studies where either a preliminary grouping was applied or one or more measured points were used. The largest

Table 4
Typical examples of the water retention PTF accuracy

Source	Pressure head (kPa)	RMSE (m^3m^{-3})	PTF input variables
Ahuja et al., 1985	−33	0.05	Clay, silt, organic matter, bulk density
	−1500	0.05	
Beke and McCormic, 1985	−33	0.05	Clay, silt, organic matter, bulk density
	−1500	0.04	
Bell, 1993	−1500	0.04	Organic matter, sand
Boix Fayos, 1997	−10	0.03	Organic matter, aggregates 0.1–1 mm.
	−1500	0.05	Organic matter, aggregates 1−2 mm, fine silt
Bruand et al., 1996	−33	0.03	Bulk density
	−1500	0.03	
Calhoun et al., 1972	−1500	0.05	Clay
Gupta and Larson, 1979	−1500	0.05	Clay, silt, organic matter content, bulk density
Koekkoek and Bootlink, 1999	−10	0.05	Sand, clay, silt, organic matter content, bulk density
	−1500	0.05	
Lenhardt, 1984	−33	0.07	Clay
	−1500	0.05	
Mayr and Jarvis, 1999	A[a]	0.03	
		0.06[b]	
Minasny et al., 1999	−33	0.07	Clay, silt, sand, bulk density, porosity, mean particle diameter, geometric standard deviation
	−1500	0.07	
Pachepsky et al., 1996	−33	0.02	Sand, silt, clay, bulk density
	−1500	0.02	
Paydar and Cresswell, 1996	A	0.02	Slope of the particle size distribution curve + one measured point on the WRC
		0.04[c]	
Paydar and Cresswell, 1996	A	0.03	Clay, silt, coarse sand, fine sand, organic matter content
		0.05[c]	
Schaap et al., 1998	A	0.11	Textural class only
Schaap et al., 1998	A	0.09	Sand, silt, clay, bulk density
Schaap and Leij, 1998	A	0.10	Sand, silt, clay
Sinowski et al., 1997	−30	0.04	Clay, silt, sand, bulk density, porosity, median particle diameter and standard deviation
	−1500	0.04	
Tomasella and Hodnett, 1998	A	0.06	Clay, silt, sand

[a] A-average RSME along the measured water retention curves obtained after estimating parameters of a water retention equation and using this equation to compute water contents at all suction where the water retention was measured.
[b] Various genetic groups.
[c] Various textural classes.

RMSE value of 0.11 $m^3 m^{-3}$ is obtained in a study where the textural class was the sole predictor. Accuracy of predicting a complete characteristic is lower than accuracy of the prediction for a specific pressure head. A clear trend of dependence of accuracy on pressure head cannot be established with only two pressure heads being evaluated. Authors who tried to observe such a trend reported the lowest accuracy somewhere between −10 and −100 kPa (Rajkai and Várallyay, 1992).

The RMSE of log(Ksat) predictions is not better than 0.5 $m^3 m^{-3}$ (Jaynes and Tyler, 1984; Ahuja et al., 1989; Tietje and Hennings, 1996; Schaap et al., 1998). The highest accuracy was attained using the Brooks and Corey water retention parameters along with basic soil properties (Timlin et al., 1999; Pachepsky et al., 1999).

Accuracy predictions are important when PTFs are to be developed for coefficients in equations and a choice of equations has to be made from the host of formulae used in literature. El-Kadi (1985a) compared several equations using mean square error of water content at several pressure heads and found Brutsaert's equation to be most accurate. Bache et al. (1981) found that a loglinear water retention equation is appropriate for loamy soils whereas it does not perform well for predominantly sandy or clayey soils. Schaap and Leij (1998) reported an RMSE of 0.10 $m^3 m^{-3}$ in approximating water retention curves in their database with the Van Genuchten Eq. (6).

The accuracy predictions themselves may serve as benchmarks. However, they should be compared to variability in other measured input data. In general, models should not be more accurate than data used in model development. Therefore, PTFs can be considered to be sufficient accurate if the variability of PTF errors does not differ significantly from variability in other data and if the average error does not significantly differ from zero. In general, variability in hydraulic characteristics depends on the extent of the area studied, on the spatial variability of soils within the area, and on the methods used for sampling and measurement.

10.2. Reliability of pedotransfer functions

The reliability of PTFs can be evaluated by cross-validation, i.e. splitting the available data set in a development and validation subset, or by using an independent data set.

With cross-validation (Hjorth, 1994), PTF reliability can be assessed by (1) drawing a random subsample from the data set, (2) developing a PTF for the subsample, and (3) testing the accuracy of the PTF against data left after subsampling. This process is repeated several times. There are several cross-validation techniques suitable for PTF development (Good, 1999). They include: (a) *K*-folding, when the data are subdivided into *K* roughly equal sizes, then the modelling process is repeated *K* times, leaving one section out each time for validation purposes; (b) *K*-folding with $K = 1$ which is called the 'leave-one-out' approach; (c) jacknife, when the left out number can range from one observation to half of the sample; (d) '*d*-delete', when a random percentage of observations is set aside for validation purposes while the remaining $100 - d\%$ are used as a training set; (e) bootstrap when a copy of the validation sample remains in the training set. Examples of the bootstrap technique are presented by Schaap et al. (1998) and of the jacknife technique by Williams et al. (1998) and Pachepsky and Rawls (1999).

Many studies assessed reliability of PTFs by applying them to independent, regional data sets. Although no general conclusion could be derived from a review of these studies, some observations can be made. PTFs developed from regional databases give good results in regions with a similar soil and landscape history. For example, water retention PTFs developed in Belgium (Vereecken et al., 1989) gave accurate predictions for soils in Northern Germany when compared with predictions by 13 other PTFs (Tietje and Tapkenhinrichs, 1993). Water retention PTFs developed for the Hungarian Plain (Pachepsky et al., 1982a) were applicable to the Caucasian Piedmont Plain (Nikolaeva et al., 1986) and for Chernozemic soils in a German data set (Tietje and Tapkenhinrichs, 1993). PTFs developed in Australia were more accurate for the Mississippi Delta when compared with other regional PTFs (Timlin et al., 1996). It remains to be seen whether this observation holds for other cases, and which soil and landscape features have to be similar in two regions to assure the mutual reliability of developed PTFs.

There are indications that the larger the differences

in soil and climatic conditions the larger the differences in PTFs that may be expected. Kay et al. (1997) found that changes in structural characteristics as predicted by their PTFs, which were derived from databases from different geographical regions of the world, exhibit considerable variation. These authors remarked that impacts of soil and climatic conditions on these PTFs have received little attention and merit more research. MacLean and Yager (1972) and Tomasella and Hodnett (1998) clearly proved the point of regional specificity of PTFs by demonstrating that PTFs developed in temperate regions do not perform well in tropical soils.

11. Dealing with uncertainty in pedotransfer function predictions in practise

A study by Finke et al. (1996) is used as an example of how can be dealt with uncertainty in model input parameters, including uncertainty in pedotransfer function predictions, when the functional behaviour of soils is simulated. For a soil mapping unit in the Netherlands, they quantified and statistically evaluated the contribution to the explanation of variability in modelling results of two major sources of uncertainty in model input parameters. The two sources of uncertainty were: (i) spatial variability of basic soil properties such as profile composition, soil texture and water-table depths; and (ii) uncertainty associated with the use of pedotransfer functions to predict soil hydraulic characteristics. When pedotransfer functions are used, the spatial variability of the basic soil properties is directly translated to variations in hydraulic characteristics and, subsequently, to variations in simulated functional soil behaviour. In addition, the prediction error of the pedotransfer function itself results in variations in the predicted soil hydraulic characteristics. This also contributes to uncertainties in simulated functional soil behaviour.

Spatial variability of soil properties within the soil mapping unit was expressed by selecting a statistically representative set of 88 profiles within the mapping unit. Uncertainty in pedotransfer function predictions was quantified by drawing 20 error terms from the covariance matrix of differences between measured and predicted soil hydraulic characteristics using a Cholesky decomposition. Adding the 20 error terms to the hydraulic characteristic directly predicted with the PTF, resulted in a set of 20 new hydraulic characteristics. As such this set quantifies the uncertainty involved in applying the PTF. As a result, $88 \times 20 = 1760$ possible combinations of soil profiles and hydraulic characteristics were generated. These combinations were used in a Monte Carlo procedure to calculate the following functional aspects of soil behaviour 'days with good workability', 'days with sufficient aeration', 'chloride breakthrough', 'cadmium breakthrough' and 'isoproturon breakthrough'. The contribution of the two sources of uncertainty to the explanation of variability in modelling results of the 5 functional aspects of soil behaviour were statistically evaluated by an analysis of variance.

Fig. 5 shows that uncertainty in pedotransfer functions plays an important role when functional aspects of soil behaviour with a physical nature are calculated, such as 'days with good workability' and 'sufficient aeration'. If adsorbing chemicals, such as 'cadmium breakthrough' and 'isoproturon breakthrough', are considered the uncertainty caused by variability in basic soil properties largely explains the uncertainty in the modelling results. In case of the inert tracer, 'chloride breakthrough' modelling results are far less sensitive to variability in basic soil properties when compared to the adsorbing chemicals cadmium and isoproturon. This is understandable because variability in basic soil properties means essentially variability in percentages clay, silt and organic matter. In turn, these variabilities have a large influence on the adsorption of cadmium and isoproturon.

This example illustrates that there is not a single source of variability, either PTF-related or soil-related, that can explain the uncertainty in every calculated functional aspect of soil behaviour. Contrarily, depending on the type of functional aspect of soil behaviour one is interested in, variability in different types of input parameters will dominate uncertainty in results. As a consequence, it is rewarding to first identify which type of input parameter dominates the explanation of uncertainty in results. Next, the variability of this type of input parameters can be assessed and possibly be reduced. An analysis along these lines will also help to indicate whether the use of

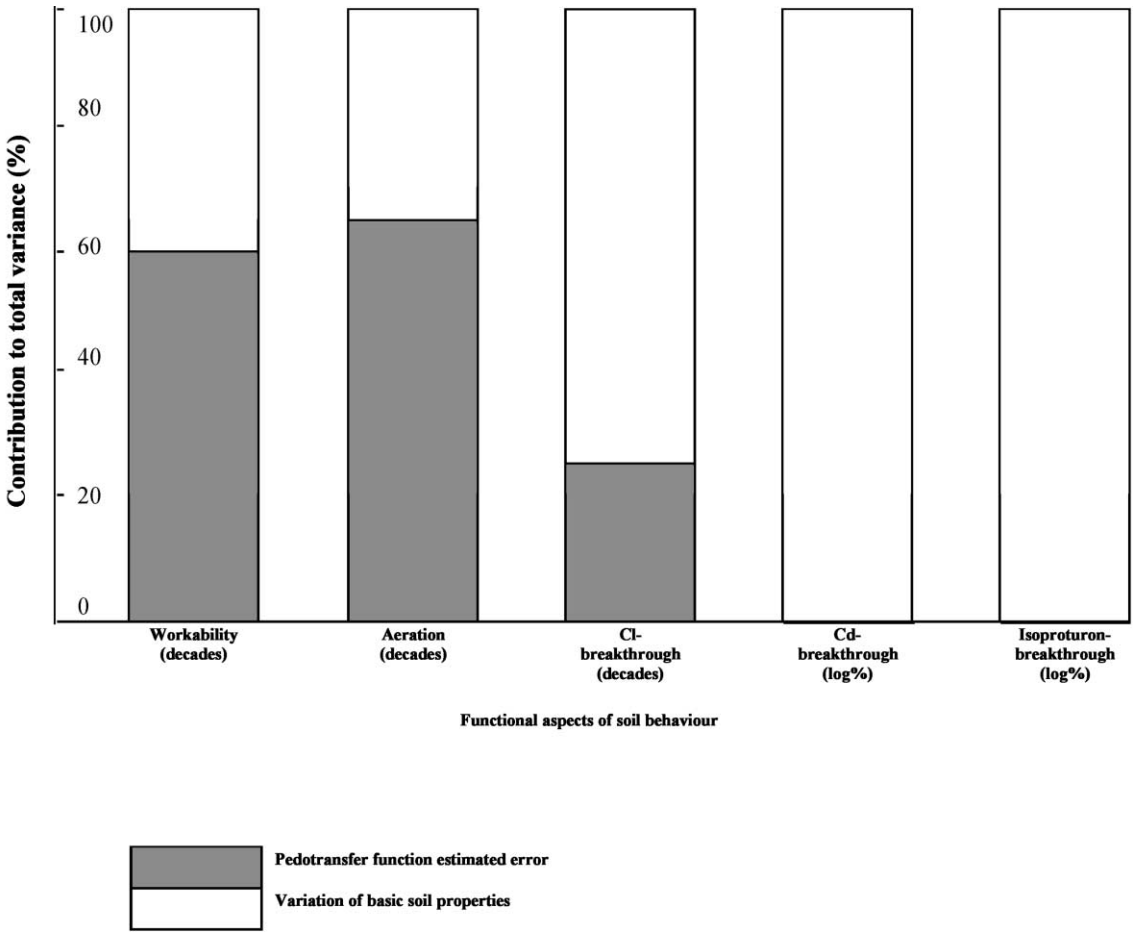

Fig. 5. Relative importance of different sources of variability in explaining the uncertainty in five simulated functional aspects of soil behaviour (after Finke et al., 1996).

an existing PTF and its associated uncertainty is sufficiently accurate to generate the soil hydraulic characteristics for a specific application or if additional, costly soil physical measurements are justified.

The described study is an example of a functional evaluation of PTFs which was first proposed by Wösten et al. (1986) who used criteria directly related to applications rather than statistics to characterize the accuracy. Vereecken et al. (1992) defined functional evaluation as the statistical examination of the variability in the outcome of a simulation model for a specific application when the variability arises solely from uncertainty in the PTFs. Vereecken et al. (1992) found that prediction errors in hydraulic characteristics account for about 90% of variations in moisture supply capacity of soil. The remaining 10% are due to the within map variability. These authors presented the seemingly paradoxical case study in which errors of PTFs with better accuracy result in higher variability in simulated moisture supply capacity and in simulated downward fluxes beyond the root zone.

At least four factors affect the performance of a PTF in simulations. These are the accuracy of basic soil data used as inputs in PTFs, the accuracy of PTF itself, specific features of the simulation model, and the output used as a functional criteria. Workman and Scaggs (1992) compared performance of PTFs in two models, PREFLO and DRAINMOD, in simulations of evapotranspiration, infiltration, runoff and drainage. PREFLO was more sensitive than DRAINMOD to

predictions of the saturated water content. Differences between measured and PTF predicted hydraulic characteristics created larger differences in model output than differences in the two models.

When the sensitivity of a model to hydraulic characteristics is not substantial, the accuracy of PTF may not be an issue. Wopereis et al. (1993) presented a functional evaluation of PTF predicted hydraulic conductivity for simulating water content in the upper 40 cm soil layer under dryland rice cultivation. Although PTF predicted hydraulic conductivity differed substantially from measured values, good agreement was obtained between observed and simulated soil water contents, just because simulation results were relatively insensitive to this parameter. A similar conclusion was reached by Wösten et al. (1995) when they compared the functional behavior of hydraulic characteristics predicted with class and continuous PTFs. The simulated number of workable days did not depend on the type of pedotransfer function applied whereas the number of days with good aeration did.

Functional evaluation of PTFs can be done without taking into account PTF accuracy per se. Wösten et al. (1990a) compared the performance of four different PTFs in the same model and found in an analysis of variance no significant differences in terms of simulating soil water content in the upper 50 cm soil layer. In this case, PTF cost rather than its accuracy was used as a criterion. Verburg et al. (1996) applied four different PTFs to predict parameters for water and bromide transport in soil profiles, and found that differences in PTF predictions did not affect bromide transport simulations with their model. Functional evaluation showed that differences in PTF performance in modeling studies may depend on other environmental variables. No difference was found between performance of several PTFs when only the type of PTF was considered as input for the analysis of variance (Wösten et al., 1990b). However, when the same data were re-analysed using rainfall deficit as a co-variable, the analysis of variance showed a clear effect of the type of PTF.

Data collected at different scales may be available for the functional evaluation of PTFs. Including scale information in the PTF evaluation process involves the following three operations: interpolation, running the model and aggregation of results (Heuvelink and Pebesma, 1999). In principle, it is possible to aggregate first and to simulate later, or alternatively to simulate first and to aggregate later. Heuvelink (1998) recommends to run the model in many points at small scale within a large scale resolution unit and then to aggregate simulation results.

The majority of PTFs are developed from measurements on standard small samples. Soil sample size may affect both average values of soil hydraulic characteristics as well as their spatial distributions (Shein et al., 1995; Giménez et al., 1999; Pachepsky et al., 2001b). Such scale effects, albeit documented, are still not understood to the extent that scale can be incorporated in PTFs. Therefore, local application of PTFs developed at the sample scale remains a typical feature of its use.

12. Conclusions

Based on the review of the literature on pedotransfer functions a number of conclusions can be formulated.

- Pedotransfer functions are a powerful tool in predicting physical and chemical properties of soils. Because PTFs predict missing characteristics from already available basic soil data, they have the clear advantage that they are relatively inexpensive and easy to derive and to use.
- For application at a specific point, prediction with a PTF might be inadequate. In the latter case, direct measurement is the only option. PTFs should not be used to make predictions for soils that are outside the range of soils used to derive the PTFs. In other words use of PTFs for interpolation purposes is safe whereas they are not recommended to be used for extrapolation.
- Development of PTFs requires large and reliable databases. This implies that well structured and easily accessible national and international databases of measured soil hydraulic characteristics need to be created. PTFs should be periodically updated as more measured data become available from these databases.
- Research on PTFs is stimulated by expanding the types of properties stored in databases. Among these properties are: (a) detailed particle size

analysis with at least five to nine classes, (b) clay mineralogy, bulk density and organic matter content, (c) morphological information, (d) chemical properties, and (e) distribution of pore sizes and their continuity with depth. Factors that have shown to be influential need to be characterized with more detail in databases.

- The accuracy and reliability of pedotransfer functions may be appropriated for many applications on regional and national scale. On these scales temporal and spatial variability of other than hydraulic characteristics most likely will also have an important impact on the modelling results.
- The search for data mining tools to develop better (more flexible) PTFs and the search for additional soil properties as inputs in PTFs are important directions for improving PTF accuracy and reliability. However, the accurate measurement of hydraulic characteristics is probably the most important factor for future progress.
- Quantification of uncertainty in PTFs is useful. Evaluation of its effects on calculated functional aspects of soil behaviour will show which input parameter need to be known in more detail to arrive at more accurate results.

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